A redesign of light-driven rotary molecular motors

Pollard, Michael M.; Meetsma, Auke; Feringa, Ben L.

Published in:
Organic and Biomolecular Chemistry

DOI:
10.1039/b715652a

Publication date:
2008

```
data_global

#==============================================================================
_journal_coden_Cambridge         177
# 0. AUDIT DETAILS

_audit_creation_date             '2006-06-07 15:58:08'
_audit_creation_method
;
PLATON <TABLE ACC> option (version :: 40506)
SHELXL97-2 & Manual Editing
;
_audit_update_record
;
?
;

#==============================================================================

# 1. SUBMISSION DETAILS

_publ_contact_author_name        # Name of author for correspondence
;
Drs. A. Meetsma
;
_publ_contact_author_address     # Address of author for correspondence
;
Crystal Structure Center,
Chemical Physics,
Materials Science Center,
University of Groningen,
Nijenborgh 4,
NL-9747 AG Groningen,
The Netherlands.
;
_publ_contact_author_email       A.Meetsma@rug.nl
_publ_contact_author_fax         '+31 50 3634441'
_publ_contact_author_phone       '+31 50 3634368'

_publ_requested_journal          'Chem. Comm.'
# Publication choise FI, CI or EI for Inorganic
# FM, CM or EM for Metal-organic
# FO, CO or EO for Organic
_publ_requested_category         ?
_publ_requested_coeditor_name    ?

_publ_contact_letter             # Include date of submission
;
Date of submission : 2007-08-06 11:58:08

Consider this CIF submission for deposition of the first
X-ray structure of a manuscript to be submitted to : Chem. Comm
(Our Compound_Identification_Code : Q1117)
;

loop_
_publ_author_name
```

B.Feringa
A.Meetsma
M.Pollard

_publ_section_exptl_refinement
;
The structure was solved by direct methods using the program SIR2004.
The positional and anisotropic displacement parameters for the
non-hydrogen atoms were refined. A subsequent difference Fourier
synthesis resulted in the location of all the hydrogen atoms,
which coordinates and isotropic displacement parameters were refined.
;

Insert blank lines between references

_publ_section_references
;
Allen, F.H. (2000). Acta Cryst. B58, 380-388.

Bondi, A. (1964). J. Phys. Chem. 68, 441-451.

Bruker, (2000). SMART, SAINTPLUS and XPREP.
Software Reference Manual Bruker AXS Inc. Madison, Wisconsin, USA.

Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G.L.,
De Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005).
SIR2004. An improved tool for crystal structure determination and
refinement. J. Appl. Cryst. 38, 381-388.

Hahn, T. (1983). Ed. International Tables for Crystallography,
Volume A, Space-group symmetry, Kluwer Academic Publishers,
Dordrecht, The Netherlands.

Le Page, Y. (1987). J. Appl. Cryst. 20, 264-269.

Le Page, Y. (1988). J. Appl. Cryst. 21, 983-984.

Meetsma, A. (2005). Extended version of the program PLUTO.
University of Groningen, The Netherlands. (unpublished).

Sheldrick, G.M. (1997). SHELXL-97. Program for Crystal Structure
Refinement. University of G\"ottingen, Germany.

Sheldrick, G.M. (2001). SADABS. Version 2.03.
Multi-Scan Absorption Correction Program.
University of G\"ottingen, Germany.

Spek, A.L. (1987). Acta Cryst. C43, 1233-1235.

Spek, A.L. (1988). J. Appl. Cryst. 21, 578-579.

Spek, A.L. (1990). Acta Cryst. A46, C-34.

Spek, A.L. (2003). J. Appl. Cryst. 36, 7-13.

Wilson, A.J.C. (1992). Ed. International Tables for Crystallography,
Volume C, Kluwer Academic Publishers, Dordrecht, The Netherlands.
;

_publ_section_figure_captions
;

Fig. 1. Perspective PLUTO drawing of the molecule illustrating the configuration and the adopted numbering scheme.

Fig. 2. Molecular packing viewed down unit cell axes.

Fig. 3. Perspective ORTEP drawing of the title compound. Displacement ellipsoids for non-H are represented at the 50% probability level.
The H-atoms are drawn with an arbitrary radius.
;

#===
data_1
_database_code_depnum_ccdc_archive 'CCDC 666199'
5. CHEMICAL DATA

_chemical_name_systematic
;
;
_chemical_name_common   ?
_chemical_melting_point   ?
_chemical_formula_moiety   'C24 H28'
Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_structural   ?
_chemical_formula_sum   'C24 H28'
_chemical_formula_iupac   ?
_chemical_formula_weight   316.48
_chemical_compound_source   'see text'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#===

6. CRYSTAL DATA

_symmetry_cell_setting   Triclinic
_symmetry_space_group_name_Hall '-P 1'
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number   2

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z

_cell_length_a   11.4202(7)
_cell_length_b   13.2038(8)
_cell_length_c   13.6607(8)
_cell_angle_alpha   106.538(1)
_cell_angle_beta   90.402(1)
_cell_angle_gamma   115.040(1)
_cell_volume   1769.71(19)
_cell_formula_units_Z   4

```
_cell_measurement_temperature    100(1)
_cell_measurement_reflns_used    6549
_cell_measurement_theta_min      2.35
_cell_measurement_theta_max      29.55
_cell_special_details
;
The final unit cell was obtained from the xyz centroids of
6549 reflections after integration using the SAINTPLUS
software package (Bruker, 2000).

Reduced cell calculations did not indicate any higher metric lattice symmetry
and examination of the finalatomic coordinates of the structure did not
yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)
;

_exptl_crystal_description       block
_exptl_crystal_colour            colorless
_exptl_crystal_size_max          0.57
_exptl_crystal_size_mid          0.52
_exptl_crystal_size_min          0.44
_exptl_crystal_size_rad          ?
_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffrn    1.188
_exptl_crystal_density_method    'not measured'
_exptl_crystal_F_000             688
_exptl_absorpt_coefficient_mu    0.066
_exptl_absorpt_correction_type   Multi-Scan
_exptl_absorpt_process_details   '(SADABS, Sheldrick, Bruker, 2001))'
_exptl_absorpt_correction_T_min  0.959
_exptl_absorpt_correction_T_max  0.9714

#===============================================================================

# 7. EXPERIMENTAL DATA

_exptl_special_details
;
;
_diffrn_ambient_temperature      100(1)
_diffrn_radiation_wavelength     0.71073
_diffrn_radiation_type           MoK\a
_diffrn_radiation_source         'fine focus sealed Siemens Mo tube '
_diffrn_radiation_monochromator  'parallel mounted graphite'
_diffrn_radiation_detector
;
CCD area-detector
;
_diffrn_measurement_device_type
;
Bruker Smart Apex; CCD area detector
;
_diffrn_measurement_method       '\f and \w scans'
_diffrn_special_details
;
Crystal into the cold nitrogen stream of the low-temparature unit
(KRYOFLEX, (Bruker, 2000)).
;
_diffrn_detector_area_resol_mean '4096x4096 / 62x62 (binned 512)'

_diffrn_standards_number         0
```

```
_diffrn_standards_interval_count ?
_diffrn_standards_interval_time  ?
_diffrn_standards_decay_%        0

loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number            16214
_diffrn_reflns_av_R_equivalents  0.0203
_diffrn_reflns_av_sigmaI/netI    0.0365
_diffrn_reflns_limit_h_min       -15
_diffrn_reflns_limit_h_max       15
_diffrn_reflns_limit_k_min       -17
_diffrn_reflns_limit_k_max       17
_diffrn_reflns_limit_l_min       -18
_diffrn_reflns_limit_l_max       18
_diffrn_reflns_theta_min         2.71
_diffrn_reflns_theta_max         28.28
_diffrn_measured_fraction_theta_max 0.959
_diffrn_reflns_theta_full        25.00
_diffrn_measured_fraction_theta_full 0.983

_diffrn_reflns_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to F~o~^2^
using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
_reflns_number_total             8438
_reflns_number_gt                6985
_reflns_threshold_expression     I>2\s(I)

_computing_data_collection       'SMART, Version 5.624, (Bruker, 2001)'
_computing_cell_refinement       'SAINTPLUS, Version 6.02A, (Bruker, 2000)'
_computing_data_reduction        'XPREP, Version 5.1/NT, (Bruker, 2000)'
_computing_structure_solution
;
SIR2004 (Burla et al., 2005)
;
_computing_structure_refinement  'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 2006)
PLATON (Spek, 2003)
;
_computing_publication_material  'PLATON (Spek, 2003)'

#===============================================================================

# 8. REFINEMENT DATA

_refine_special_details
;
Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F^2^, conventional R-factors R are based
```

```
on F, with F set to zero for negative F^2^. The threshold expression of
F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type           full
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.0604P)^2^+0.7021P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary     direct
_atom_sites_solution_secondary   direct
_atom_sites_solution_hydrogens   geom
_refine_ls_hydrogen_treatment    refall
_refine_ls_extinction_method     none
_refine_ls_extinction_coef       ?
_refine_ls_abs_structure_details ?
_chemical_absolute_configuration ?

_refine_ls_abs_structure_Flack   ?
_refine_ls_number_reflns         8438
_refine_ls_number_parameters     657
_refine_ls_number_restraints     0
_refine_ls_number_constraints    ?
_refine_ls_R_factor_all          0.0612
_refine_ls_R_factor_gt           0.0496
_refine_ls_wR_factor_ref         0.1240
_refine_ls_wR_factor_gt          0.1176
_refine_ls_goodness_of_fit_ref   1.033
_refine_ls_restrained_S_all      1.033
_refine_ls_shift/su_max          0.000
_refine_ls_shift/su_mean         0.000

_refine_diff_density_max         0.353
_refine_diff_density_min         -0.314
_refine_diff_density_rms         0.056

_vrn_publ_code_frame_time_sec    5.0
_vrn_publ_code_meas_time_hour    6.8

#===============================================================================

# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_thermal_displace_type
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags

C11 C Uani 0.21758(12) 0.28717(11) 0.41419(10) 1.000 0.0135(3) . .
C12 C Uani 0.08547(13) 0.27385(12) 0.44638(10) 1.000 0.0143(3) . .
C13 C Uani -0.01071(13) 0.17175(12) 0.35228(10) 1.000 0.0152(4) . .
```

```
C14 C Uani 0.06524(13) 0.18869(11) 0.26311(10) 1.000 0.0149(4) . .
C15 C Uani 0.01551(13) 0.14088(12) 0.15831(11) 1.000 0.0170(4) . .
C16 C Uani 0.10335(14) 0.17639(12) 0.08983(11) 1.000 0.0183(4) . .
C17 C Uani 0.23303(14) 0.25834(13) 0.12604(11) 1.000 0.0182(4) . .
C18 C Uani 0.28492(13) 0.30439(12) 0.23115(10) 1.000 0.0154(4) . .
C19 C Uani 0.19931(13) 0.26419(11) 0.30001(10) 1.000 0.0141(3) . .
C110 C Uani 0.06643(14) 0.38527(13) 0.45859(11) 1.000 0.0179(4) . .
C111 C Uani -0.12661(15) 0.05567(13) 0.12031(12) 1.000 0.0213(4) . .
C112 C Uani 0.42511(14) 0.39701(13) 0.26444(12) 1.000 0.0182(4) . .
C113 C Uani 0.31358(12) 0.28509(11) 0.47139(10) 1.000 0.0133(3) . .
C114 C Uani 0.42584(12) 0.26082(11) 0.42903(10) 1.000 0.0137(4) . .
C115 C Uani 0.41536(13) 0.15965(12) 0.47056(11) 1.000 0.0147(4) . .
C116 C Uani 0.36423(12) 0.18761(11) 0.57178(10) 1.000 0.0143(4) . .
C117 C Uani 0.36881(13) 0.14537(12) 0.65364(11) 1.000 0.0169(4) . .
C118 C Uani 0.32291(13) 0.18959(12) 0.74276(11) 1.000 0.0186(4) . .
C119 C Uani 0.27902(13) 0.27450(13) 0.74982(11) 1.000 0.0182(4) . .
C120 C Uani 0.27189(12) 0.31616(12) 0.66712(10) 1.000 0.0152(4) . .
C121 C Uani 0.31097(12) 0.26756(11) 0.57516(10) 1.000 0.0133(3) . .
C122 C Uani 0.55958(13) 0.36738(12) 0.47378(11) 1.000 0.0161(4) . .
C123 C Uani 0.42461(15) 0.05886(13) 0.64839(13) 1.000 0.0221(4) . .
C124 C Uani 0.23019(14) 0.41335(13) 0.68343(11) 1.000 0.0178(4) . .
H12 H Uiso 0.0720(14) 0.2535(12) 0.5119(12) 1.000 0.010(3) . .
H13 H Uiso -0.0301(16) 0.0936(15) 0.3606(13) 1.000 0.021(4) . .
H13' H Uiso -0.0952(16) 0.1758(14) 0.3419(12) 1.000 0.017(4) . .
H16 H Uiso 0.0713(16) 0.1431(15) 0.0133(14) 1.000 0.024(4) . .
H17 H Uiso 0.2887(16) 0.2847(14) 0.0762(13) 1.000 0.022(4) . .
H110 H Uiso 0.1352(18) 0.4558(16) 0.5098(14) 1.000 0.029(5) . .
H110' H Uiso -0.0202(16) 0.3754(14) 0.4805(13) 1.000 0.020(4) . .
H110" H Uiso 0.0719(16) 0.4036(14) 0.3914(13) 1.000 0.022(4) . .
H111 H Uiso -0.1501(19) -0.0156(17) 0.1409(15) 1.000 0.035(5) . .
H111' H Uiso -0.1473(19) 0.0273(17) 0.0433(16) 1.000 0.037(5) . .
H111" H Uiso -0.184(2) 0.0901(17) 0.1499(15) 1.000 0.040(5) . .
H112 H Uiso 0.4866(17) 0.3612(15) 0.2536(14) 1.000 0.028(5) . .
H112' H Uiso 0.4398(16) 0.4455(14) 0.3394(14) 1.000 0.022(4) . .
H112" H Uiso 0.4464(17) 0.4499(16) 0.2216(14) 1.000 0.029(5) . .
H114 H Uiso 0.4143(14) 0.2361(13) 0.3526(12) 1.000 0.011(4) . .
H115 H Uiso 0.3525(16) 0.0811(15) 0.4228(13) 1.000 0.021(4) . .
H115' H Uiso 0.5011(16) 0.1584(14) 0.4806(13) 1.000 0.020(4) . .
H118 H Uiso 0.3244(16) 0.1605(14) 0.8020(13) 1.000 0.023(4) . .
H119 H Uiso 0.2518(17) 0.3067(15) 0.8145(14) 1.000 0.024(4) . .
H122 H Uiso 0.5650(15) 0.4408(14) 0.4630(12) 1.000 0.019(4) . .
H122' H Uiso 0.6310(16) 0.3516(14) 0.4412(13) 1.000 0.022(4) . .
H122" H Uiso 0.5784(16) 0.3860(14) 0.5518(14) 1.000 0.021(4) . .
H123 H Uiso 0.522(2) 0.0985(19) 0.6544(16) 1.000 0.046(6) . .
H123' H Uiso 0.394(2) -0.0061(18) 0.5824(16) 1.000 0.039(5) . .
H123" H Uiso 0.401(2) 0.0241(19) 0.7039(17) 1.000 0.051(6) . .
H124 H Uiso 0.2656(16) 0.4606(15) 0.6362(13) 1.000 0.023(4) . .
H124' H Uiso 0.2628(18) 0.4686(16) 0.7568(15) 1.000 0.032(5) . .
H124" H Uiso 0.1333(18) 0.3822(16) 0.6733(14) 1.000 0.029(5) . .
C21 C Uani 0.27671(12) 0.71101(11) 0.02841(10) 1.000 0.0125(3) . .
C22 C Uani 0.41188(12) 0.72836(11) 0.06756(10) 1.000 0.0133(3) . .
C23 C Uani 0.50202(13) 0.83108(12) 0.02870(11) 1.000 0.0149(4) . .
C24 C Uani 0.42211(12) 0.80839(11) -0.07105(10) 1.000 0.0139(4) . .
C25 C Uani 0.46702(13) 0.85215(11) -0.15229(11) 1.000 0.0152(4) . .
C26 C Uani 0.37672(13) 0.80918(12) -0.24129(11) 1.000 0.0161(4) . .
C27 C Uani 0.24892(13) 0.72550(12) -0.24872(11) 1.000 0.0162(4) . .
C28 C Uani 0.20117(12) 0.68486(11) -0.16579(10) 1.000 0.0137(3) . .
C29 C Uani 0.28970(12) 0.73081(11) -0.07452(10) 1.000 0.0131(3) . .
C210 C Uani 0.43476(14) 0.61931(12) 0.01835(11) 1.000 0.0175(4) . .
C211 C Uani 0.60766(14) 0.93923(12) -0.14534(12) 1.000 0.0182(4) . .
C212 C Uani 0.06155(13) 0.59188(12) -0.18105(11) 1.000 0.0165(4) . .
```

```
C213 C Uani 0.18287(12) 0.71341(11) 0.08761(10) 1.000 0.0124(3) . .
C214 C Uani 0.06866(12) 0.73654(11) 0.05888(10) 1.000 0.0130(3) . .
C215 C Uani 0.07975(13) 0.83751(11) 0.15635(11) 1.000 0.0148(4) . .
C216 C Uani 0.13449(12) 0.81070(11) 0.24209(10) 1.000 0.0140(4) . .
C217 C Uani 0.13154(12) 0.85282(11) 0.34742(11) 1.000 0.0159(4) . .
C218 C Uani 0.17968(13) 0.80920(12) 0.41214(11) 1.000 0.0176(4) . .
C219 C Uani 0.22541(13) 0.72588(12) 0.37205(11) 1.000 0.0170(4) . .
C220 C Uani 0.23167(12) 0.68494(11) 0.26651(10) 1.000 0.0144(4) . .
C221 C Uani 0.18887(12) 0.73195(11) 0.20119(10) 1.000 0.0128(3) . .
C222 C Uani -0.06498(13) 0.63026(12) 0.04484(11) 1.000 0.0162(4) . .
C223 C Uani 0.07618(14) 0.93946(13) 0.38895(12) 1.000 0.0208(4) . .
C224 C Uani 0.27735(14) 0.59024(12) 0.22956(11) 1.000 0.0165(4) . .
H22 H Uiso 0.4271(15) 0.7490(13) 0.1437(12) 1.000 0.014(4) . .
H23 H Uiso 0.5201(15) 0.9104(14) 0.0804(12) 1.000 0.016(4) . .
H23' H Uiso 0.5879(16) 0.8310(14) 0.0170(13) 1.000 0.022(4) . .
H26 H Uiso 0.4043(17) 0.8363(15) -0.3004(13) 1.000 0.025(4) . .
H27 H Uiso 0.1900(16) 0.6938(14) -0.3154(13) 1.000 0.021(4) . .
H210 H Uiso 0.3698(18) 0.5474(16) 0.0318(14) 1.000 0.029(5) . .
H210' H Uiso 0.5226(17) 0.6333(15) 0.0467(13) 1.000 0.023(4) . .
H210" H Uiso 0.4325(17) 0.6033(15) -0.0594(14) 1.000 0.026(4) . .
H211 H Uiso 0.6377(18) 1.0053(16) -0.0788(15) 1.000 0.030(5) . .
H211' H Uiso 0.6164(18) 0.9752(16) -0.2018(14) 1.000 0.031(5) . .
H211" H Uiso 0.6650(18) 0.9015(16) -0.1513(14) 1.000 0.029(5) . .
H212 H Uiso 0.0003(17) 0.6280(15) -0.1703(14) 1.000 0.028(5) . .
H212' H Uiso 0.0499(16) 0.5470(14) -0.1314(13) 1.000 0.021(4) . .
H212" H Uiso 0.0367(16) 0.5365(15) -0.2543(14) 1.000 0.024(4) . .
H214 H Uiso 0.0800(15) 0.7609(13) -0.0030(12) 1.000 0.013(4) . .
H215 H Uiso -0.0064(16) 0.8379(14) 0.1676(12) 1.000 0.016(4) . .
H215' H Uiso 0.1418(15) 0.9170(14) 0.1519(12) 1.000 0.016(4) . .
H218 H Uiso 0.1796(16) 0.8374(15) 0.4875(14) 1.000 0.023(4) . .
H219 H Uiso 0.2526(16) 0.6926(14) 0.4199(12) 1.000 0.018(4) . .
H222 H Uiso -0.0823(16) 0.6148(14) 0.1134(14) 1.000 0.023(4) . .
H222' H Uiso -0.0715(15) 0.5564(14) -0.0068(13) 1.000 0.018(4) . .
H222" H Uiso -0.1357(17) 0.6472(15) 0.0203(13) 1.000 0.025(4) . .
H223 H Uiso 0.1123(18) 1.0057(16) 0.3620(14) 1.000 0.029(5) . .
H223' H Uiso 0.0987(19) 0.9743(17) 0.4665(16) 1.000 0.037(5) . .
H223" H Uiso -0.0214(19) 0.9015(16) 0.3702(14) 1.000 0.033(5) . .
H224 H Uiso 0.3773(17) 0.6241(15) 0.2370(13) 1.000 0.024(4) . .
H224' H Uiso 0.2434(16) 0.5454(14) 0.1551(13) 1.000 0.020(4) . .
H224" H Uiso 0.2501(18) 0.5372(16) 0.2721(14) 1.000 0.031(5) . .

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
C11 0.0136(6) 0.0132(6) 0.0150(6) 0.0053(5) 0.0039(5) 0.0066(5)
C12 0.0136(6) 0.0176(6) 0.0139(6) 0.0056(5) 0.0022(5) 0.0085(5)
C13 0.0134(6) 0.0175(6) 0.0159(7) 0.0058(5) 0.0014(5) 0.0076(5)
C14 0.0168(6) 0.0153(6) 0.0159(7) 0.0055(5) 0.0026(5) 0.0099(5)
C15 0.0200(7) 0.0164(6) 0.0174(7) 0.0038(5) 0.0002(5) 0.0118(5)
C16 0.0252(7) 0.0233(7) 0.0124(7) 0.0036(5) 0.0013(5) 0.0177(6)
C17 0.0238(7) 0.0245(7) 0.0152(7) 0.0089(5) 0.0072(5) 0.0171(6)
C18 0.0180(7) 0.0170(6) 0.0167(7) 0.0065(5) 0.0042(5) 0.0120(5)
C19 0.0165(6) 0.0157(6) 0.0136(6) 0.0048(5) 0.0021(5) 0.0103(5)
C110 0.0169(7) 0.0204(7) 0.0196(7) 0.0060(6) 0.0023(5) 0.0114(6)
C111 0.0206(7) 0.0208(7) 0.0198(8) 0.0011(6) -0.0022(6) 0.0102(6)
C112 0.0180(7) 0.0207(7) 0.0201(7) 0.0100(6) 0.0066(5) 0.0101(6)
```

```
C113 0.0137(6) 0.0123(6) 0.0136(6) 0.0036(5) 0.0028(5) 0.0059(5)
C114 0.0136(6) 0.0152(6) 0.0137(7) 0.0045(5) 0.0023(5) 0.0078(5)
C115 0.0139(6) 0.0152(6) 0.0162(7) 0.0045(5) 0.0014(5) 0.0079(5)
C116 0.0102(6) 0.0138(6) 0.0159(7) 0.0043(5) 0.0001(5) 0.0030(5)
C117 0.0117(6) 0.0164(6) 0.0203(7) 0.0072(5) -0.0026(5) 0.0034(5)
C118 0.0137(6) 0.0234(7) 0.0174(7) 0.0114(6) -0.0002(5) 0.0040(5)
C119 0.0125(6) 0.0245(7) 0.0148(7) 0.0060(5) 0.0022(5) 0.0059(5)
C120 0.0099(6) 0.0173(6) 0.0162(7) 0.0046(5) 0.0008(5) 0.0044(5)
C121 0.0092(6) 0.0143(6) 0.0144(6) 0.0050(5) 0.0005(5) 0.0032(5)
C122 0.0132(6) 0.0171(6) 0.0180(7) 0.0048(5) 0.0034(5) 0.0071(5)
C123 0.0228(8) 0.0193(7) 0.0268(8) 0.0104(6) -0.0012(6) 0.0098(6)
C124 0.0169(7) 0.0212(7) 0.0159(7) 0.0040(5) 0.0039(5) 0.0102(5)
C21 0.0111(6) 0.0118(6) 0.0138(6) 0.0032(5) -0.0004(5) 0.0050(5)
C22 0.0103(6) 0.0168(6) 0.0127(6) 0.0037(5) 0.0008(5) 0.0066(5)
C23 0.0107(6) 0.0169(6) 0.0159(7) 0.0044(5) 0.0019(5) 0.0056(5)
C24 0.0140(6) 0.0140(6) 0.0148(7) 0.0029(5) 0.0023(5) 0.0083(5)
C25 0.0156(6) 0.0139(6) 0.0185(7) 0.0045(5) 0.0053(5) 0.0092(5)
C26 0.0200(7) 0.0176(6) 0.0164(7) 0.0080(5) 0.0064(5) 0.0118(5)
C27 0.0186(7) 0.0175(6) 0.0150(7) 0.0038(5) 0.0013(5) 0.0113(5)
C28 0.0143(6) 0.0138(6) 0.0147(6) 0.0039(5) 0.0024(5) 0.0081(5)
C29 0.0143(6) 0.0140(6) 0.0140(6) 0.0048(5) 0.0037(5) 0.0088(5)
C210 0.0161(7) 0.0194(7) 0.0204(7) 0.0057(5) 0.0035(5) 0.0114(5)
C211 0.0154(7) 0.0176(7) 0.0230(8) 0.0084(6) 0.0062(5) 0.0072(5)
C212 0.0143(6) 0.0178(6) 0.0156(7) 0.0041(5) 0.0001(5) 0.0062(5)
C213 0.0113(6) 0.0111(5) 0.0145(6) 0.0044(5) 0.0002(5) 0.0046(5)
C214 0.0117(6) 0.0150(6) 0.0145(6) 0.0062(5) 0.0029(5) 0.0070(5)
C215 0.0120(6) 0.0140(6) 0.0192(7) 0.0058(5) 0.0034(5) 0.0062(5)
C216 0.0092(6) 0.0126(6) 0.0178(7) 0.0045(5) 0.0026(5) 0.0030(5)
C217 0.0109(6) 0.0149(6) 0.0176(7) 0.0024(5) 0.0027(5) 0.0036(5)
C218 0.0129(6) 0.0211(7) 0.0135(7) 0.0028(5) 0.0025(5) 0.0045(5)
C219 0.0123(6) 0.0214(7) 0.0160(7) 0.0076(5) 0.0008(5) 0.0054(5)
C220 0.0100(6) 0.0155(6) 0.0159(7) 0.0051(5) 0.0012(5) 0.0040(5)
C221 0.0088(6) 0.0135(6) 0.0136(6) 0.0035(5) 0.0013(4) 0.0032(5)
C222 0.0114(6) 0.0167(6) 0.0196(7) 0.0059(5) 0.0013(5) 0.0054(5)
C223 0.0169(7) 0.0197(7) 0.0221(8) 0.0006(6) 0.0037(6) 0.0087(6)
C224 0.0168(7) 0.0186(6) 0.0176(7) 0.0073(5) 0.0021(5) 0.0100(5)

#===============================================================================

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
Bond distances, angles etc. have been calculated using the
rounded fractional coordinates. All su's are estimated
from the variances of the (full) variance-covariance matrix.
The cell esds are taken into account in the estimation of
distances, angles and torsion angles
;

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
C11 C12 1.526(2) . . no
C11 C19 1.4970(18) . . no
C11 C113 1.356(2) . . no
C12 C13 1.555(2) . . no
```

C12 C110 1.540(2) . . no
C13 C14 1.514(2) . . no
C14 C19 1.415(2) . . no
C14 C15 1.3933(19) . . no
C15 C16 1.402(2) . . no
C15 C111 1.510(2) . . no
C16 C17 1.392(2) . . no
C17 C18 1.403(2) . . no
C18 C19 1.407(2) . . no
C18 C112 1.510(2) . . no
C12 H12 1.000(16) . . no
C113 C121 1.4985(19) . . no
C13 H13' 1.00(2) . . no
C113 C114 1.528(2) . . no
C13 H13 1.000(19) . . no
C114 C115 1.555(2) . . no
C114 C122 1.538(2) . . no
C115 C116 1.514(2) . . no
C116 C117 1.394(2) . . no
C16 H16 1.009(18) . . no
C116 C121 1.415(2) . . no
C117 C118 1.400(2) . . no
C117 C123 1.512(2) . . no
C17 H17 0.971(18) . . no
C118 C119 1.390(2) . . no
C119 C120 1.406(2) . . no
C120 C124 1.510(2) . . no
C120 C121 1.4073(19) . . no
C110 H110' 1.00(2) . . no
C110 H110" 1.010(17) . . no
C110 H110 0.99(2) . . no
C111 H111' 1.00(2) . . no
C111 H111" 0.98(2) . . no
C111 H111 0.99(2) . . no
C112 H112' 1.010(18) . . no
C112 H112" 0.99(2) . . no
C112 H112 0.99(2) . . no
C114 H114 0.991(16) . . no
C115 H115' 1.00(2) . . no
C115 H115 0.997(18) . . no
C118 H118 0.993(17) . . no
C119 H119 0.980(19) . . no
C21 C29 1.4989(19) . . no
C21 C213 1.353(2) . . no
C21 C22 1.530(2) . . no
C122 H122' 1.002(19) . . no
C122 H122" 1.023(18) . . no
C22 C210 1.537(2) . . no
C122 H122 0.998(18) . . no
C22 C23 1.555(2) . . no
C123 H123' 0.99(2) . . no
C123 H123" 0.98(2) . . no
C123 H123 1.00(3) . . no
C23 C24 1.516(2) . . no
C124 H124 0.994(18) . . no
C124 H124" 1.00(2) . . no
C24 C25 1.397(2) . . no
C24 C29 1.414(2) . . no
C124 H124' 1.01(2) . . no
C25 C26 1.399(2) . . no
C25 C211 1.511(2) . . no

```
C26 C27 1.389(2) . . no
C27 C28 1.406(2) . . no
C28 C29 1.4061(19) . . no
C28 C212 1.512(2) . . no
C22 H22 0.991(16) . . no
C23 H23 1.016(17) . . no
C23 H23' 1.00(2) . . no
C26 H26 0.976(18) . . no
C27 H27 0.997(18) . . no
C213 C214 1.532(2) . . no
C213 C221 1.4967(18) . . no
C214 C215 1.553(2) . . no
C214 C222 1.538(2) . . no
C215 C216 1.517(2) . . no
C216 C217 1.3935(19) . . no
C216 C221 1.414(2) . . no
C217 C218 1.402(2) . . no
C217 C223 1.509(2) . . no
C218 C219 1.389(2) . . no
C219 C220 1.4023(19) . . no
C220 C224 1.512(2) . . no
C220 C221 1.409(2) . . no
C210 H210' 0.99(2) . . no
C210 H210" 1.020(18) . . no
C210 H210 1.00(2) . . no
C211 H211' 1.000(19) . . no
C211 H211" 0.97(2) . . no
C211 H211 1.00(2) . . no
C212 H212' 0.996(17) . . no
C212 H212" 1.010(18) . . no
C212 H212 0.99(2) . . no
C214 H214 0.978(16) . . no
C215 H215' 1.007(18) . . no
C215 H215 1.00(2) . . no
C218 H218 0.990(18) . . no
C219 H219 0.997(18) . . no
C222 H222' 1.000(17) . . no
C222 H222" 1.00(2) . . no
C222 H222 1.018(18) . . no
C223 H223' 1.01(2) . . no
C223 H223" 1.00(2) . . no
C223 H223 0.98(2) . . no
C224 H224' 0.996(17) . . no
C224 H224" 0.99(2) . . no
C224 H224 1.03(2) . . no

loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
C12 C11 C19 104.78(12) . . . no
C12 C11 C113 125.24(12) . . . no
C19 C11 C113 127.38(13) . . . no
C11 C12 C13 101.69(11) . . . no
C11 C12 C110 112.32(12) . . . no
C13 C12 C110 109.46(12) . . . no
```

```
C12 C13 C14 102.85(12) . . . no
C13 C14 C15 127.08(14) . . . no
C13 C14 C19 110.48(11) . . . no
C15 C14 C19 122.43(13) . . . no
C14 C15 C16 116.89(14) . . . no
C14 C15 C111 121.56(14) . . . no
C16 C15 C111 121.55(13) . . . no
C15 C16 C17 121.00(13) . . . no
C16 C17 C18 122.47(14) . . . no
C17 C18 C19 116.90(14) . . . no
C17 C18 C112 119.08(13) . . . no
C19 C18 C112 123.95(12) . . . no
C11 C19 C14 107.01(12) . . . no
C11 C19 C18 133.06(13) . . . no
C14 C19 C18 119.90(12) . . . no
C13 C12 H12 112.0(9) . . . no
C110 C12 H12 109.0(9) . . . no
C11 C12 H12 112.3(10) . . . no
C114 C113 C121 104.79(12) . . . no
C14 C13 H13 110.5(10) . . . no
C14 C13 H13' 111.7(9) . . . no
C12 C13 H13' 112.7(9) . . . no
C11 C113 C114 125.06(12) . . . no
C11 C113 C121 127.61(13) . . . no
C12 C13 H13 110.6(10) . . . no
H13 C13 H13' 108.5(15) . . . no
C113 C114 C122 112.14(11) . . . no
C115 C114 C122 109.07(12) . . . no
C113 C114 C115 101.69(11) . . . no
C114 C115 C116 102.75(12) . . . no
C17 C16 H16 119.7(11) . . . no
C115 C116 C121 110.50(12) . . . no
C117 C116 C121 122.50(13) . . . no
C15 C16 H16 119.3(11) . . . no
C115 C116 C117 126.99(13) . . . no
C118 C117 C123 121.21(13) . . . no
C116 C117 C118 116.89(14) . . . no
C116 C117 C123 121.88(13) . . . no
C16 C17 H17 118.2(11) . . . no
C18 C17 H17 119.4(11) . . . no
C117 C118 C119 121.17(14) . . . no
C118 C119 C120 122.35(14) . . . no
C119 C120 C121 116.97(14) . . . no
C121 C120 C124 124.16(13) . . . no
C119 C120 C124 118.80(12) . . . no
C113 C121 C120 133.01(13) . . . no
C116 C121 C120 119.84(12) . . . no
C113 C121 C116 107.11(12) . . . no
C12 C110 H110' 111.3(10) . . . no
C12 C110 H110" 110.5(10) . . . no
C12 C110 H110 112.2(12) . . . no
H110' C110 H110" 108.7(15) . . . no
H110' C110 H110 108.0(16) . . . no
H110" C110 H110 105.9(15) . . . no
C15 C111 H111' 112.4(13) . . . no
C15 C111 H111" 111.6(13) . . . no
C15 C111 H111 110.7(13) . . . no
H111' C111 H111" 109.4(18) . . . no
H111' C111 H111 105.9(17) . . . no
H111" C111 H111 106.5(18) . . . no
C18 C112 H112' 110.9(11) . . . no
```

C18 C112 H112" 109.4(12) . . . no
C18 C112 H112 111.5(11) . . . no
H112' C112 H112" 109.0(15) . . . no
H112' C112 H112 109.5(15) . . . no
H112" C112 H112 106.5(16) . . . no
C113 C114 H114 111.7(10) . . . no
C115 C114 H114 112.0(10) . . . no
C122 C114 H114 110.1(10) . . . no
C114 C115 H115' 112.3(10) . . . no
C114 C115 H115 111.4(11) . . . no
C116 C115 H115' 111.9(10) . . . no
C116 C115 H115 110.5(11) . . . no
H115' C115 H115 108.1(15) . . . no
C117 C118 H118 118.5(11) . . . no
C119 C118 H118 120.3(11) . . . no
C118 C119 H119 119.2(11) . . . no
C120 C119 H119 118.4(11) . . . no
C22 C21 C29 104.70(12) . . . no
C22 C21 C213 125.22(12) . . . no
C29 C21 C213 127.35(13) . . . no
C114 C122 H122' 110.7(10) . . . no
C114 C122 H122" 110.7(10) . . . no
C114 C122 H122 112.9(10) . . . no
C21 C22 C23 101.15(11) . . . no
C21 C22 C210 112.47(12) . . . no
C23 C22 C210 109.61(12) . . . no
H122' C122 H122 107.5(15) . . . no
H122" C122 H122 106.2(14) . . . no
H122' C122 H122" 108.6(15) . . . no
H123' C123 H123" 107.8(19) . . . no
H123' C123 H123 105.8(19) . . . no
C117 C123 H123' 112.8(14) . . . no
C117 C123 H123" 110.8(15) . . . no
C117 C123 H123 110.9(14) . . . no
C22 C23 C24 102.73(12) . . . no
H123" C123 H123 108.5(19) . . . no
C120 C124 H124' 109.8(12) . . . no
C120 C124 H124" 112.0(12) . . . no
C120 C124 H124 112.1(11) . . . no
H124' C124 H124" 106.7(17) . . . no
H124' C124 H124 107.9(15) . . . no
H124" C124 H124 108.1(16) . . . no
C23 C24 C25 127.42(13) . . . no
C23 C24 C29 110.43(12) . . . no
C25 C24 C29 122.13(13) . . . no
C24 C25 C26 116.93(14) . . . no
C24 C25 C211 121.42(13) . . . no
C26 C25 C211 121.63(13) . . . no
C25 C26 C27 121.33(13) . . . no
C26 C27 C28 122.15(13) . . . no
C27 C28 C29 116.98(13) . . . no
C27 C28 C212 118.76(12) . . . no
C29 C28 C212 124.20(12) . . . no
C21 C29 C24 106.88(12) . . . no
C21 C29 C28 132.94(13) . . . no
C24 C29 C28 120.12(12) . . . no
C23 C22 H22 112.5(10) . . . no
C210 C22 H22 108.9(10) . . . no
C21 C22 H22 112.1(11) . . . no
C22 C23 H23 110.9(10) . . . no
C24 C23 H23 111.4(10) . . . no

```
C24 C23 H23' 111.7(10) . . . no
C22 C23 H23' 112.7(10) . . . no
H23 C23 H23' 107.4(15) . . . no
C25 C26 H26 119.7(12) . . . no
C27 C26 H26 119.0(12) . . . no
C26 C27 H27 118.2(11) . . . no
C28 C27 H27 119.6(11) . . . no
C214 C213 C221 104.92(11) . . . no
C21 C213 C221 127.77(13) . . . no
C21 C213 C214 124.84(12) . . . no
C213 C214 C222 112.82(12) . . . no
C215 C214 C222 108.66(12) . . . no
C213 C214 C215 101.76(11) . . . no
C214 C215 C216 102.65(11) . . . no
C215 C216 C217 126.89(13) . . . no
C215 C216 C221 110.69(11) . . . no
C217 C216 C221 122.41(13) . . . no
C216 C217 C223 121.12(13) . . . no
C218 C217 C223 121.89(13) . . . no
C216 C217 C218 116.97(13) . . . no
C217 C218 C219 121.08(13) . . . no
C218 C219 C220 122.41(14) . . . no
C219 C220 C221 117.04(13) . . . no
C221 C220 C224 124.37(12) . . . no
C219 C220 C224 118.53(13) . . . no
C213 C221 C220 133.04(13) . . . no
C216 C221 C220 119.85(12) . . . no
C213 C221 C216 107.07(12) . . . no
C22 C210 H210' 110.1(11) . . . no
C22 C210 H210" 110.4(11) . . . no
C22 C210 H210 112.8(12) . . . no
H210' C210 H210" 107.1(16) . . . no
H210' C210 H210 107.2(17) . . . no
H210" C210 H210 109.2(15) . . . no
C25 C211 H211' 109.7(12) . . . no
C25 C211 H211" 111.3(12) . . . no
C25 C211 H211 111.3(12) . . . no
H211' C211 H211" 108.9(17) . . . no
H211' C211 H211 106.8(16) . . . no
H211" C211 H211 108.6(17) . . . no
C28 C212 H212' 111.0(11) . . . no
C28 C212 H212" 109.6(11) . . . no
C28 C212 H212 111.0(11) . . . no
H212' C212 H212" 110.2(15) . . . no
H212' C212 H212 107.8(16) . . . no
H212" C212 H212 107.1(16) . . . no
C213 C214 H214 110.5(11) . . . no
C215 C214 H214 112.2(10) . . . no
C222 C214 H214 110.7(10) . . . no
C214 C215 H215' 111.4(9) . . . no
C214 C215 H215 112.4(9) . . . no
C216 C215 H215' 110.4(10) . . . no
C216 C215 H215 111.9(9) . . . no
H215' C215 H215 108.1(15) . . . no
C217 C218 H218 119.3(11) . . . no
C219 C218 H218 119.6(11) . . . no
C218 C219 H219 118.7(10) . . . no
C220 C219 H219 118.9(10) . . . no
C214 C222 H222' 113.0(11) . . . no
C214 C222 H222" 109.8(11) . . . no
C214 C222 H222 109.9(11) . . . no
```

```
H222' C222 H222" 107.4(15) . . . no
H222' C222 H222 108.1(14) . . . no
H222" C222 H222 108.6(15) . . . no
C217 C223 H223' 111.1(13) . . . no
C217 C223 H223" 111.6(12) . . . no
C217 C223 H223 111.6(13) . . . no
H223' C223 H223" 108.6(17) . . . no
H223' C223 H223 106.2(16) . . . no
H223" C223 H223 107.5(17) . . . no
C220 C224 H224' 110.7(11) . . . no
C220 C224 H224" 110.1(12) . . . no
C220 C224 H224 112.5(11) . . . no
H224' C224 H224" 111.1(15) . . . no
H224' C224 H224 106.8(15) . . . no
H224" C224 H224 105.5(16) . . . no

loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
C19 C11 C12 C13 36.11(14) . . . . no
C19 C11 C12 C110 -80.80(13) . . . . no
C113 C11 C12 C13 -126.66(14) . . . . no
C113 C11 C12 C110 116.42(15) . . . . no
C12 C11 C19 C14 -27.39(15) . . . . no
C12 C11 C19 C18 150.66(17) . . . . no
C113 C11 C19 C14 134.89(15) . . . . no
C113 C11 C19 C18 -47.1(3) . . . . no
C12 C11 C113 C114 160.32(13) . . . . no
C12 C11 C113 C121 1.2(2) . . . . no
C19 C11 C113 C114 1.4(2) . . . . no
C19 C11 C113 C121 -157.69(14) . . . . no
C11 C12 C13 C14 -31.30(14) . . . . no
C110 C12 C13 C14 87.67(14) . . . . no
C12 C13 C14 C15 -162.96(15) . . . . no
C12 C13 C14 C19 15.98(16) . . . . no
C13 C14 C15 C16 175.14(14) . . . . no
C13 C14 C15 C111 -4.3(2) . . . . no
C19 C14 C15 C16 -3.7(2) . . . . no
C19 C14 C15 C111 176.86(14) . . . . no
C13 C14 C19 C11 6.75(16) . . . . no
C13 C14 C19 C18 -171.61(13) . . . . no
C15 C14 C19 C11 -174.25(14) . . . . no
C15 C14 C19 C18 7.4(2) . . . . no
C14 C15 C16 C17 -1.9(2) . . . . no
C111 C15 C16 C17 177.59(15) . . . . no
C15 C16 C17 C18 3.9(3) . . . . no
C16 C17 C18 C19 -0.2(2) . . . . no
C16 C17 C18 C112 -177.32(15) . . . . no
C17 C18 C19 C11 176.93(16) . . . . no
C17 C18 C19 C14 -5.2(2) . . . . no
C112 C18 C19 C11 -6.1(3) . . . . no
C112 C18 C19 C14 171.76(14) . . . . no
C29 C21 C22 C23 37.18(13) . . . . no
```

```
C29 C21 C22 C210 -79.67(14) . . . . no
C213 C21 C22 C23 -125.17(15) . . . . no
C213 C21 C22 C210 117.98(15) . . . . no
C22 C21 C29 C24 -27.70(15) . . . . no
C22 C21 C29 C28 149.26(16) . . . . no
C213 C21 C29 C24 134.14(15) . . . . no
C213 C21 C29 C28 -48.9(2) . . . . no
C22 C21 C213 C214 158.88(13) . . . . no
C22 C21 C213 C221 -0.6(2) . . . . no
C29 C21 C213 C214 0.5(2) . . . . no
C29 C21 C213 C221 -158.90(14) . . . . no
C21 C22 C23 C24 -32.69(13) . . . . no
C210 C22 C23 C24 86.24(14) . . . . no
C22 C23 C24 C25 -160.92(14) . . . . no
C22 C23 C24 C29 17.37(15) . . . . no
C23 C24 C25 C26 173.64(14) . . . . no
C23 C24 C25 C211 -4.7(2) . . . . no
C29 C24 C25 C26 -4.5(2) . . . . no
C29 C24 C25 C211 177.24(14) . . . . no
C23 C24 C29 C21 6.08(16) . . . . no
C23 C24 C29 C28 -171.35(13) . . . . no
C25 C24 C29 C21 -175.53(13) . . . . no
C25 C24 C29 C28 7.0(2) . . . . no
C24 C25 C26 C27 -1.0(2) . . . . no
C211 C25 C26 C27 177.34(14) . . . . no
C25 C26 C27 C28 3.9(2) . . . . no
C26 C27 C28 C29 -1.4(2) . . . . no
C26 C27 C28 C212 -178.81(14) . . . . no
C27 C28 C29 C21 179.45(15) . . . . no
C27 C28 C29 C24 -3.9(2) . . . . no
C212 C28 C29 C21 -3.3(3) . . . . no
C212 C28 C29 C24 173.35(14) . . . . no
C21 C213 C214 C215 -127.71(14) . . . . no
C21 C213 C214 C222 116.04(15) . . . . no
C221 C213 C214 C215 35.59(13) . . . . no
C221 C213 C214 C222 -80.65(13) . . . . no
C21 C213 C221 C216 136.57(15) . . . . no
C21 C213 C221 C220 -45.8(2) . . . . no
C214 C213 C221 C216 -26.08(15) . . . . no
C214 C213 C221 C220 151.58(16) . . . . no
C213 C214 C215 C216 -31.53(13) . . . . no
C222 C214 C215 C216 87.71(14) . . . . no
C214 C215 C216 C217 -161.38(14) . . . . no
C214 C215 C216 C221 17.12(15) . . . . no
C215 C216 C217 C218 175.35(14) . . . . no
C215 C216 C217 C223 -3.4(2) . . . . no
C221 C216 C217 C218 -3.0(2) . . . . no
C221 C216 C217 C223 178.28(14) . . . . no
C215 C216 C221 C213 5.27(16) . . . . no
C215 C216 C221 C220 -172.75(13) . . . . no
C217 C216 C221 C213 -176.15(13) . . . . no
C217 C216 C221 C220 5.8(2) . . . . no
C216 C217 C218 C219 -1.4(2) . . . . no
C223 C217 C218 C219 177.37(15) . . . . no
C217 C218 C219 C220 2.9(2) . . . . no
C218 C219 C220 C221 -0.1(2) . . . . no
C218 C219 C220 C224 -177.37(14) . . . . no
C219 C220 C221 C213 178.50(15) . . . . no
C219 C220 C221 C216 -4.1(2) . . . . no
C224 C220 C221 C213 -4.4(3) . . . . no
C224 C220 C221 C216 172.97(14) . . . . no
```

```
loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
_geom_contact_publ_flag
C11 C124 3.553(2) . . no
C12 C120 3.447(2) . . no
C12 C124 3.250(2) . . no
C12 C218 3.548(2) . 2_566 no
C16 C214 3.535(2) . 2_565 no
C18 C114 3.440(2) . . no
C21 C224 3.549(2) . . no
C22 C220 3.452(2) . . no
C22 C224 3.249(2) . . no
C22 C118 3.546(2) . 2_666 no
C28 C214 3.4529(19) . . no
C110 C124 3.428(2) . . no
C11 H112' 2.935(19) . . no
C12 H124" 2.957(18) . . no
C12 H218 3.03(2) . 2_566 no
C112 C113 3.555(2) . . no
C112 C114 3.256(2) . . no
C112 C122 3.431(2) . . no
C12 H124 3.005(18) . . no
C112 C124 3.588(2) . 2_666 no
C13 H111 3.09(2) . . no
C13 H223 3.09(2) . 1_545 no
C13 H218 2.922(19) . 2_566 no
C13 H111" 3.02(2) . . no
C113 C112 3.555(2) . . no
C14 H110" 2.848(18) . . no
C114 C18 3.440(2) . . no
C114 C112 3.256(2) . . no
C15 H212 3.09(2) . 2_565 no
C16 H111' 3.03(2) . 2_555 no
C16 H214 2.910(18) . 2_565 no
C16 H222" 3.017(19) . 2_565 no
C17 H222" 3.058(19) . 2_565 no
C17 H211" 2.90(2) . 2_665 no
C18 H211" 2.92(2) . 2_665 no
C18 H114 2.774(17) . . no
C118 C22 3.546(2) . 2_666 no
C19 H114 2.753(17) . . no
C19 H110" 2.837(19) . . no
C120 C12 3.447(2) . . no
C21 H224' 3.063(18) . . no
C21 H212' 2.940(18) . . no
C22 H118 3.016(19) . 2_666 no
C22 H224 2.962(18) . . no
C22 H224' 2.951(18) . . no
C122 C112 3.431(2) . . no
C23 H211 2.96(2) . . no
C23 H118 2.982(18) . 2_666 no
C124 C12 3.250(2) . . no
C24 H211 3.05(2) . 2_675 no
C24 H210" 2.809(19) . . no
C124 C11 3.553(2) . . no
C124 C110 3.428(2) . . no
```

C124 C112 3.588(2) . 2_666 no
C25 H112 3.03(2) . 2_665 no
C25 H23 2.945(18) . 2_675 no
C26 H114 3.018(17) . 2_665 no
C26 H122' 2.917(17) . 2_665 no
C26 H123" 3.04(2) . 1_564 no
C27 H13' 3.041(19) . 2_565 no
C27 H111" 2.82(2) . 2_565 no
C27 H122' 3.089(18) . 2_665 no
C28 H111" 3.01(2) . 2_565 no
C28 H214 2.796(17) . . no
C29 H214 2.732(18) . . no
C29 H210" 2.84(2) . . no
C210 C224 3.438(2) . . no
C110 H124 2.947(18) . . no
C110 H124" 3.041(19) . . no
C111 H13' 2.929(16) . . no
C211 C215 3.579(2) . 2_675 no
C111 H16 3.051(19) . 2_555 no
C212 C224 3.518(2) . 2_565 no
C112 H114 2.686(16) . . no
C212 C214 3.271(2) . . no
C212 C213 3.558(2) . . no
C112 H122 2.917(16) . . no
C212 C222 3.415(2) . . no
C213 C212 3.558(2) . . no
C113 H112' 3.073(18) . . no
C113 H124 2.977(18) . . no
C114 H26 3.06(2) . 2_665 no
C214 C28 3.4529(19) . . no
C214 C16 3.535(2) . 2_565 no
C114 H112' 2.974(18) . . no
C214 C212 3.271(2) . . no
C114 H112 3.006(19) . . no
C215 C211 3.579(2) . 2_675 no
C115 H123' 2.94(2) . . no
C116 H223' 3.10(2) . 1_545 no
C116 H122" 2.813(18) . . no
C118 H210' 3.076(18) . 2_666 no
C118 H22 2.911(18) . 2_666 no
C218 C12 3.548(2) . 2_566 no
C119 H223" 2.95(2) . 2_566 no
C120 H12 2.780(16) . . no
C220 C22 3.452(2) . . no
C120 H223" 2.98(2) . 2_566 no
C121 H122" 2.851(19) . . no
C121 H12 2.771(17) . . no
C122 H219 3.064(19) . 2_666 no
C122 H124 3.090(19) . 2_666 no
C122 H112 3.085(18) . . no
C122 H112' 2.923(19) . . no
C222 C212 3.415(2) . . no
C122 H112' 3.002(18) . 2_666 no
C123 H22 3.093(16) . 2_666 no
C123 H115' 2.918(17) . . no
C224 C21 3.549(2) . . no
C124 H12 2.666(16) . . no
C224 C210 3.438(2) . . no
C124 H110 2.890(19) . . no
C224 C212 3.518(2) . 2_565 no
C224 C22 3.249(2) . . no

C210 H224 3.051(17) . . no
C210 H224' 2.917(18) . . no
C211 H114 3.034(16) . 2_665 no
C211 H23' 2.924(17) . . no
C211 H23 2.885(18) . 2_675 no
C211 H215' 2.702(18) . 2_675 no
C212 H222' 2.877(17) . . no
C212 H214 2.729(16) . . no
C213 H224' 2.950(18) . . no
C213 H222' 3.071(18) . 2_565 no
C213 H212' 3.075(17) . . no
C214 H212' 2.983(17) . . no
C214 H16 3.01(2) . 2_565 no
C214 H212 2.988(18) . . no
C215 H223 2.949(19) . . no
C215 H16 3.011(19) . 2_565 no
C216 H222 2.800(18) . . no
C217 H115 2.876(19) . 1_565 no
C218 H123' 3.00(2) . 1_565 no
C218 H12 2.922(17) . 2_566 no
C219 H123 2.94(2) . 2_666 no
C220 H123 2.94(2) . 2_666 no
C220 H22 2.788(17) . . no
C221 H222 2.874(19) . . no
C221 H22 2.772(18) . . no
C222 H212 3.032(19) . . no
C222 H212' 2.970(18) . 2_565 no
C222 H119 3.10(2) . 2_566 no
C222 H224' 3.051(17) . 2_565 no
C222 H212' 2.913(18) . . no
C223 H115 2.86(2) . 1_565 no
C223 H13 2.88(2) . 1_565 no
C223 H12 3.088(15) . 2_566 no
C223 H215 2.900(16) . . no
C224 H22 2.662(17) . . no
C224 H210 2.900(19) . . no
H110' H13' 2.55(2) . . no
H110" C14 2.848(18) . . no
H110" C19 2.837(19) . . no
H111' H16 2.42(3) . . no
H111' C16 3.03(2) . 2_555 no
H111" C13 3.02(2) . . no
H111" H13' 2.55(3) . . no
H111" C27 2.82(2) . 2_565 no
H111" C28 3.01(2) . 2_565 no
H112' C11 2.935(19) . . no
H112' C113 3.073(18) . . no
H112' C114 2.974(18) . . no
H112' C122 2.923(19) . . no
H112' C122 3.002(18) . 2_666 no
H112' H122" 2.39(3) . 2_666 no
H112' H122 2.24(3) . . no
H112" H17 2.47(3) . . no
H115' C123 2.918(17) . . no
H115' H122' 2.57(3) . . no
H122' C26 2.917(17) . 2_665 no
H122' C27 3.089(18) . 2_665 no
H122' H115' 2.57(3) . . no
H122' H26 2.54(3) . 2_665 no
H122" C121 2.851(19) . . no
H122" H112' 2.39(3) . 2_666 no

H122" C116 2.813(18) . . no
H123' C218 3.00(2) . 1_545 no
H123' H218 2.47(3) . 1_545 no
H123' C115 2.94(2) . . no
H123" H118 2.40(3) . . no
H123" C26 3.04(2) . 1_546 no
H123" H26 2.48(3) . 1_546 no
H12 H124" 2.25(2) . . no
H12 C120 2.780(16) . . no
H12 C121 2.771(17) . . no
H12 C124 2.666(16) . . no
H12 C218 2.922(17) . 2_566 no
H12 C223 3.088(15) . 2_566 no
H124' H119 2.44(3) . . no
H13 C223 2.88(2) . 1_545 no
H13 H223 2.37(3) . 1_545 no
H13' H218 2.55(2) . 2_566 no
H13' C111 2.929(16) . . no
H13' H110' 2.55(2) . . no
H13' H111" 2.55(3) . . no
H13' H27 2.49(3) . 2_565 no
H13' C27 3.041(19) . 2_565 no
H124" H12 2.25(2) . . no
H124" C12 2.957(18) . . no
H124" C110 3.041(19) . . no
H210' H23' 2.55(3) . . no
H210' C118 3.076(17) . 2_666 no
H210" C24 2.809(19) . . no
H210" C29 2.84(2) . . no
H16 C215 3.011(19) . 2_565 no
H16 H214 2.56(3) . 2_565 no
H16 C214 3.01(2) . 2_565 no
H16 C111 3.051(19) . 2_555 no
H16 H111' 2.42(3) . . no
H211' H26 2.42(3) . . no
H211' H215' 2.49(3) . 2_675 no
H17 H23' 2.59(3) . 2_665 no
H17 H112" 2.47(3) . . no
H211" H215' 2.48(3) . 2_675 no
H211" C18 2.92(2) . 2_665 no
H211" C17 2.90(2) . 2_665 no
H212' C222 2.913(18) . . no
H212' H222' 2.21(3) . . no
H212' C222 2.970(18) . 2_565 no
H212' H222 2.39(3) . 2_565 no
H212' C214 2.983(17) . . no
H212' C21 2.940(18) . . no
H212' C213 3.075(17) . . no
H212" H27 2.45(3) . . no
H215' C211 2.702(18) . 2_675 no
H215' H211' 2.49(3) . 2_675 no
H215' H211" 2.48(3) . 2_675 no
H222' H212' 2.21(3) . . no
H222' C213 3.071(18) . 2_565 no
H222' C212 2.877(17) . . no
H222' H224' 2.43(3) . 2_565 no
H22 C123 3.093(16) . 2_666 no
H22 H118 2.57(3) . 2_666 no
H22 C118 2.911(18) . 2_666 no
H22 C220 2.788(17) . . no
H22 C221 2.772(18) . . no

H22 C224 2.662(17) . . no
H22 H224 2.25(2) . . no
H222" H215 2.55(2) . . no
H222" C16 3.017(19) . 2_565 no
H222" C17 3.058(19) . 2_565 no
H23 C211 2.885(18) . 2_675 no
H23 H211 2.49(3) . 2_675 no
H23 C25 2.945(18) . 2_675 no
H23' C211 2.924(17) . . no
H23' H210' 2.55(3) . . no
H23' H17 2.59(3) . 2_665 no
H223' C116 3.10(2) . 1_565 no
H223' H218 2.43(3) . . no
H223" C119 2.95(2) . 2_566 no
H223" C120 2.98(2) . 2_566 no
H224' C210 2.917(18) . . no
H224' C22 2.951(18) . . no
H224' C21 3.063(18) . . no
H224' C222 3.051(17) . 2_565 no
H224' H222' 2.43(3) . 2_565 no
H224' C213 2.950(18) . . no
H224' H210 2.23(3) . . no
H26 C114 3.06(2) . 2_665 no
H26 H123" 2.48(3) . 1_564 no
H26 H211' 2.42(3) . . no
H26 H122' 2.54(3) . 2_665 no
H224" H219 2.43(3) . . no
H27 H212" 2.45(3) . . no
H27 H13' 2.49(3) . 2_565 no
H110 H124 2.24(3) . . no
H110 C124 2.890(19) . . no
H111 H118 2.43(3) . 2_556 no
H111 C13 3.09(2) . . no
H112 C114 3.006(19) . . no
H112 C25 3.03(2) . 2_665 no
H112 C122 3.085(18) . . no
H112 H114 2.32(2) . . no
H114 C18 2.774(17) . . no
H114 H112 2.32(2) . . no
H114 C19 2.753(17) . . no
H114 C112 2.686(16) . . no
H114 C211 3.034(16) . 2_665 no
H114 C26 3.018(17) . 2_665 no
H115 C223 2.86(2) . 1_545 no
H115 H223 2.53(3) . 1_545 no
H115 C217 2.876(19) . 1_545 no
H118 C22 3.016(19) . 2_666 no
H118 C23 2.982(18) . 2_666 no
H118 H22 2.57(3) . 2_666 no
H118 H123" 2.40(3) . . no
H118 H111 2.43(3) . 2_556 no
H119 C222 3.10(2) . 2_566 no
H119 H124' 2.44(3) . . no
H122 C112 2.917(16) . . no
H122 H112' 2.24(3) . . no
H122 H122 2.60(3) . 2_666 no
H122 H124 2.49(3) . 2_666 no
H123 C219 2.94(2) . 2_666 no
H123 C220 2.94(2) . 2_666 no
H124 C113 2.977(18) . . no
H124 H122 2.49(3) . 2_666 no

```
H124 H110 2.24(3) . . no
H124 C122 3.090(19) . 2_666 no
H124 C12 3.005(18) . . no
H124 C110 2.947(18) . . no
H210 C224 2.900(19) . . no
H210 H224' 2.23(3) . . no
H211 C23 2.96(2) . . no
H211 C24 3.05(2) . 2_675 no
H211 H23 2.49(3) . 2_675 no
H212 C214 2.988(18) . . no
H212 C222 3.032(19) . . no
H212 H214 2.34(2) . . no
H212 C15 3.09(2) . 2_565 no
H214 C28 2.796(17) . . no
H214 C29 2.732(18) . . no
H214 C212 2.729(16) . . no
H214 H212 2.34(2) . . no
H214 C16 2.910(18) . 2_565 no
H214 H16 2.56(3) . 2_565 no
H215 C223 2.900(16) . . no
H215 H222" 2.55(2) . . no
H215 H222 2.56(2) . . no
H218 H123' 2.47(3) . 1_565 no
H218 H223' 2.43(3) . . no
H218 C12 3.03(2) . 2_566 no
H218 C13 2.922(19) . 2_566 no
H218 H13' 2.55(2) . 2_566 no
H219 H224" 2.43(3) . . no
H219 C122 3.064(19) . 2_666 no
H222 C216 2.800(18) . . no
H222 C221 2.874(19) . . no
H222 H215 2.56(2) . . no
H222 H212' 2.39(3) . 2_565 no
H223 C13 3.09(2) . 1_565 no
H223 C215 2.949(19) . . no
H223 H13 2.37(3) . 1_565 no
H223 H115 2.53(3) . 1_565 no
H224 C22 2.962(18) . . no
H224 C210 3.051(17) . . no
H224 H22 2.25(2) . . no

# Loop Mechanism for Extra Tables(s)

#loop_
#_publ_manuscript_incl_extra_item
#'_geom_extra_tableA_col_1'
#'_geom_extra_tableA_col_2'
#'_geom_extra_tableA_col_3'
#'_geom_extra_table_head_A'
#'_geom_table_footnote_A'
#'_geom_extra_tableB_col_1'
#'_geom_extra_tableB_col_2'
#'_geom_extra_tableB_col_3'
#'_geom_extra_table_head_B'
#'_geom_table_footnote_B'

#
#loop_
#_geom_extra_tableA_col_1
#_geom_extra_tableA_col_2
#_geom_extra_tableA_col_3
```

```
# ? ? ?

#
#loop_
#_geom_extra_tableB_col_1
#_geom_extra_tableB_col_2
#_geom_extra_tableB_col_3
# ? ? ?

#
#_geom_table_footnote_A
#;
# ?
#;

#
#_geom_table_footnote_B
#;
# ?
#;

#
#_geom_table_footnote_A
#;
# ?
#;

#
#_geom_table_footnote_B
#;
# ?
#;

#===END of Crystallographic Information File

# Attachment 'q1118.cif'

# CIF-file generated for C24H28 C2/c q1118
#==============================================================================
data_2
_database_code_depnum_ccdc_archive 'CCDC 666200'

# 5. CHEMICAL DATA

_chemical_name_systematic
;
;
_chemical_name_common            ?
_chemical_melting_point          ?
_chemical_formula_moiety         'C24 H28'
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_structural     ?
_chemical_formula_sum            'C24 H28'
_chemical_formula_iupac          ?
_chemical_formula_weight         316.48
_chemical_compound_source        'see text'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
```

```
_atom_type_scat_dispersion_imag
_atom_type_scat_source
H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#==============================================================================

# 6. CRYSTAL DATA

_symmetry_cell_setting           Monoclinic
_symmetry_space_group_name_Hall  '-C 2yc'
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y,1/2-z
3 -x,-y,-z
4 x,-y,1/2+z
5 1/2+x,1/2+y,z
6 1/2-x,1/2+y,1/2-z
7 1/2-x,1/2-y,-z
8 1/2+x,1/2-y,1/2+z

_cell_length_a                   38.531(9)
_cell_length_b                   5.981(1)
_cell_length_c                   16.016(4)
_cell_angle_alpha                90
_cell_angle_beta                 93.416(4)
_cell_angle_gamma                90
_cell_volume                     3684.4(14)
_cell_formula_units_Z            8

_cell_measurement_temperature    100(1)
_cell_measurement_reflns_used    7794
_cell_measurement_theta_min      2.55
_cell_measurement_theta_max      29.50
_cell_special_details
;
The final unit cell was obtained from the xyz centroids of
7794 reflections after integration using the SAINTPLUS
software package (Bruker, 2000).

Reduced cell calculations did not indicate any higher metric lattice symmetry
and examination of the finalatomic coordinates of the structure did not
yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)
;

_exptl_crystal_description       needle
_exptl_crystal_colour            colorless
_exptl_crystal_size_max          0.57
_exptl_crystal_size_mid          0.17
_exptl_crystal_size_min          0.15
_exptl_crystal_size_rad          ?
_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffrn    1.141
_exptl_crystal_density_method    'not measured'
_exptl_crystal_F_000             1376
_exptl_absorpt_coefficient_mu    0.064
```

```
_exptl_absorpt_correction_type   Multi-Scan
_exptl_absorpt_process_details   '(SADABS, Sheldrick, Bruker, 2001))'
_exptl_absorpt_correction_T_min  0.9616
_exptl_absorpt_correction_T_max  0.9905

#===============================================================================

# 7. EXPERIMENTAL DATA

_exptl_special_details
;
;
_diffrn_ambient_temperature      100(1)
_diffrn_radiation_wavelength     0.71073
_diffrn_radiation_type           MoK\a
_diffrn_radiation_source         'fine focus sealed Siemens Mo tube '
_diffrn_radiation_monochromator  'parallel mounted graphite'
_diffrn_radiation_detector
;
CCD area-detector
;
_diffrn_measurement_device_type
;
Bruker Smart Apex; CCD area detector
;
_diffrn_measurement_method       '\f and \w scans'
_diffrn_special_details
;
Crystal into the cold nitrogen stream of the low-temparature unit
(KRYOFLEX, (Bruker, 2000)).
;
_diffrn_detector_area_resol_mean '4096x4096 / 62x62 (binned 512)'

_diffrn_standards_number         0
_diffrn_standards_interval_count ?
_diffrn_standards_interval_time  ?
_diffrn_standards_decay_%        0

loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number            12897
_diffrn_reflns_av_R_equivalents  0.0375
_diffrn_reflns_av_sigmaI/netI    0.0397
_diffrn_reflns_limit_h_min       -47
_diffrn_reflns_limit_h_max       47
_diffrn_reflns_limit_k_min       -7
_diffrn_reflns_limit_k_max       7
_diffrn_reflns_limit_l_min       -19
_diffrn_reflns_limit_l_max       19
_diffrn_reflns_theta_min         2.55
_diffrn_reflns_theta_max         26.02
_diffrn_measured_fraction_theta_max 0.999
_diffrn_reflns_theta_full        25.00
_diffrn_measured_fraction_theta_full 0.999

_diffrn_reflns_reduction_process
```

```
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to F~o~^2^
using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
_reflns_number_total              3628
_reflns_number_gt                 2970
_reflns_threshold_expression      I>2\s(I)

_computing_data_collection        'SMART, Version 5.624, (Bruker, 2001)'
_computing_cell_refinement        'SAINTPLUS, Version 6.02A, (Bruker, 2000)'
_computing_data_reduction         'XPREP, Version 5.1/NT, (Bruker, 2000)'
_computing_structure_solution
;
SIR2004 (Burla et al., 2005)
;
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 2006)
PLATON (Spek, 2003)
;
_computing_publication_material   'PLATON (Spek, 2003)'

#===============================================================================

# 8. REFINEMENT DATA

_refine_special_details
;
Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F^2^, conventional R-factors R are based
on F, with F set to zero for negative F^2^. The threshold expression of
F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type           full
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.0674P)^2^+2.0136P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary     direct
_atom_sites_solution_secondary   direct
_atom_sites_solution_hydrogens   difmap
_refine_ls_hydrogen_treatment    refall
_refine_ls_extinction_method     none
_refine_ls_extinction_coef       ?
_refine_ls_abs_structure_details ?
_chemical_absolute_configuration ?

_refine_ls_abs_structure_Flack   ?
_refine_ls_number_reflns         3628
_refine_ls_number_parameters     329
_refine_ls_number_restraints     0
_refine_ls_number_constraints    ?
_refine_ls_R_factor_all          0.0566
```

```
_refine_ls_R_factor_gt           0.0451
_refine_ls_wR_factor_ref         0.1211
_refine_ls_wR_factor_gt          0.1137
_refine_ls_goodness_of_fit_ref   1.020
_refine_ls_restrained_S_all      1.020
_refine_ls_shift/su_max          0.000
_refine_ls_shift/su_mean         0.000

_refine_diff_density_max         0.262
_refine_diff_density_min         -0.195
_refine_diff_density_rms         0.044

_vrn_publ_code_frame_time_sec    20.0
_vrn_publ_code_meas_time_hour    16.3

#===============================================================================

# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_thermal_displace_type
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
C1 C Uani 0.13492(3) 0.3407(2) 0.27600(8) 1.000 0.0181(4) . .
C2 C Uani 0.14417(4) 0.4351(2) 0.19124(9) 1.000 0.0212(4) . .
C3 C Uani 0.16677(4) 0.6421(3) 0.21788(9) 1.000 0.0238(4) . .
C4 C Uani 0.18404(3) 0.5695(2) 0.30060(9) 1.000 0.0209(4) . .
C5 C Uani 0.21443(3) 0.6560(2) 0.34070(9) 1.000 0.0238(4) . .
C6 C Uani 0.22648(4) 0.5491(3) 0.41433(10) 1.000 0.0273(5) . .
C7 C Uani 0.20958(4) 0.3636(3) 0.44529(10) 1.000 0.0253(5) . .
C8 C Uani 0.17888(3) 0.2759(2) 0.40577(9) 1.000 0.0208(4) . .
C9 C Uani 0.16551(3) 0.3903(2) 0.33405(8) 1.000 0.0188(4) . .
C10 C Uani 0.16489(4) 0.2676(3) 0.14094(10) 1.000 0.0250(5) . .
C11 C Uani 0.23305(4) 0.8543(3) 0.30553(12) 1.000 0.0318(5) . .
C12 C Uani 0.16388(4) 0.0615(3) 0.43790(10) 1.000 0.0250(4) . .
C13 C Uani 0.10366(3) 0.2478(2) 0.28939(8) 1.000 0.0183(4) . .
C14 C Uani 0.07845(3) 0.1606(2) 0.21889(9) 1.000 0.0210(4) . .
C15 C Uani 0.06461(4) -0.0560(3) 0.25906(9) 1.000 0.0241(4) . .
C16 C Uani 0.06441(3) 0.0064(2) 0.35043(9) 1.000 0.0202(4) . .
C17 C Uani 0.04452(3) -0.0873(2) 0.41176(9) 1.000 0.0235(4) . .
C18 C Uani 0.04742(4) 0.0138(3) 0.49057(10) 1.000 0.0266(5) . .
C19 C Uani 0.06812(4) 0.2018(3) 0.50651(9) 1.000 0.0248(5) . .
C20 C Uani 0.08845(3) 0.2965(2) 0.44562(8) 1.000 0.0202(4) . .
C21 C Uani 0.08716(3) 0.1878(2) 0.36749(8) 1.000 0.0187(4) . .
C22 C Uani 0.04851(4) 0.3246(3) 0.19736(10) 1.000 0.0251(5) . .
C23 C Uani 0.02151(4) -0.2886(3) 0.39414(12) 1.000 0.0294(5) . .
C24 C Uani 0.10786(4) 0.5118(3) 0.46371(9) 1.000 0.0229(4) . .
H2 H Uiso 0.1236(4) 0.482(3) 0.1564(9) 1.000 0.021(4) . .
H3 H Uiso 0.1833(4) 0.683(3) 0.1745(10) 1.000 0.031(4) . .
H3' H Uiso 0.1523(4) 0.783(3) 0.2269(10) 1.000 0.034(5) . .
H6 H Uiso 0.2478(5) 0.606(3) 0.4437(11) 1.000 0.035(5) . .
H7 H Uiso 0.2189(4) 0.283(3) 0.4969(10) 1.000 0.025(4) . .
H10 H Uiso 0.1846(5) 0.212(3) 0.1762(11) 1.000 0.032(4) . .
H10' H Uiso 0.1730(4) 0.339(3) 0.0879(11) 1.000 0.029(4) . .
```

```
H10" H Uiso 0.1507(4) 0.130(3) 0.1242(10) 1.000 0.029(4) . .
H11 H Uiso 0.2412(5) 0.821(3) 0.2478(13) 1.000 0.048(5) . .
H11' H Uiso 0.2530(6) 0.903(4) 0.3459(13) 1.000 0.061(6) . .
H11" H Uiso 0.2175(5) 0.987(3) 0.2975(11) 1.000 0.039(5) . .
H12 H Uiso 0.1460(4) 0.090(3) 0.4798(11) 1.000 0.032(4) . .
H12' H Uiso 0.1830(5) -0.030(3) 0.4680(10) 1.000 0.033(4) . .
H12" H Uiso 0.1527(5) -0.030(3) 0.3916(11) 1.000 0.036(5) . .
H14 H Uiso 0.0904(4) 0.129(3) 0.1676(10) 1.000 0.020(4) . .
H15 H Uiso 0.0408(5) -0.102(3) 0.2317(11) 1.000 0.035(5) . .
H15' H Uiso 0.0809(4) -0.190(3) 0.2513(10) 1.000 0.030(4) . .
H18 H Uiso 0.0340(5) -0.050(3) 0.5357(11) 1.000 0.035(5) . .
H19 H Uiso 0.0684(4) 0.275(3) 0.5626(11) 1.000 0.030(4) . .
H22 H Uiso 0.0364(4) 0.362(3) 0.2486(10) 1.000 0.026(4) . .
H22' H Uiso 0.0322(4) 0.259(3) 0.1553(11) 1.000 0.032(4) . .
H22" H Uiso 0.0571(4) 0.471(3) 0.1718(11) 1.000 0.035(5) . .
H23 H Uiso 0.0352(5) -0.426(3) 0.3845(11) 1.000 0.040(5) . .
H23' H Uiso 0.0046(6) -0.271(4) 0.3444(15) 1.000 0.066(7) . .
H23" H Uiso 0.0069(6) -0.323(4) 0.4393(14) 1.000 0.057(6) . .
H24 H Uiso 0.0967(4) 0.601(3) 0.5066(11) 1.000 0.031(4) . .
H24' H Uiso 0.1086(4) 0.603(3) 0.4113(11) 1.000 0.034(5) . .
H24" H Uiso 0.1315(5) 0.476(3) 0.4870(11) 1.000 0.039(5) . .

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
C1 0.0170(6) 0.0169(7) 0.0203(7) -0.0009(5) 0.0004(5) 0.0025(5)
C2 0.0180(7) 0.0232(8) 0.0221(7) 0.0035(6) -0.0003(5) 0.0014(6)
C3 0.0196(7) 0.0220(8) 0.0301(8) 0.0042(6) 0.0048(6) 0.0010(6)
C4 0.0154(6) 0.0197(7) 0.0279(7) -0.0031(6) 0.0039(5) 0.0029(5)
C5 0.0137(6) 0.0219(8) 0.0362(8) -0.0076(6) 0.0043(6) 0.0016(6)
C6 0.0128(7) 0.0328(9) 0.0359(9) -0.0113(7) -0.0013(6) 0.0023(6)
C7 0.0162(7) 0.0327(9) 0.0267(8) -0.0029(6) -0.0017(6) 0.0083(6)
C8 0.0155(6) 0.0235(8) 0.0234(7) -0.0020(6) 0.0021(5) 0.0057(6)
C9 0.0137(6) 0.0198(7) 0.0228(7) -0.0036(5) 0.0014(5) 0.0022(5)
C10 0.0229(7) 0.0295(9) 0.0229(8) 0.0009(6) 0.0031(6) 0.0024(7)
C11 0.0181(7) 0.0256(9) 0.0522(11) -0.0054(8) 0.0068(7) -0.0035(7)
C12 0.0206(7) 0.0267(8) 0.0278(8) 0.0058(7) 0.0021(6) 0.0068(6)
C13 0.0173(7) 0.0165(7) 0.0208(7) -0.0012(5) -0.0003(5) 0.0026(5)
C14 0.0169(7) 0.0240(8) 0.0221(7) -0.0039(6) 0.0006(5) -0.0010(6)
C15 0.0184(7) 0.0215(8) 0.0321(8) -0.0048(6) -0.0002(6) -0.0018(6)
C16 0.0140(6) 0.0186(7) 0.0278(7) -0.0006(6) -0.0006(5) 0.0035(5)
C17 0.0137(6) 0.0214(8) 0.0355(8) 0.0058(6) 0.0017(6) 0.0041(6)
C18 0.0193(7) 0.0301(9) 0.0310(8) 0.0091(7) 0.0066(6) 0.0057(6)
C19 0.0212(7) 0.0300(9) 0.0233(8) 0.0009(6) 0.0021(6) 0.0073(6)
C20 0.0144(6) 0.0230(8) 0.0229(7) 0.0003(6) -0.0013(5) 0.0056(5)
C21 0.0123(6) 0.0193(7) 0.0243(7) 0.0025(6) -0.0005(5) 0.0035(5)
C22 0.0209(7) 0.0281(9) 0.0255(8) -0.0041(7) -0.0046(6) 0.0002(6)
C23 0.0191(8) 0.0241(9) 0.0454(10) 0.0053(7) 0.0047(7) -0.0008(6)
C24 0.0196(7) 0.0250(8) 0.0237(8) -0.0062(6) -0.0016(6) 0.0037(6)

#=============================================================================

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
```

```
Bond distances, angles etc. have been calculated using the
rounded fractional coordinates. All su's are estimated
from the variances of the (full) variance-covariance matrix.
The cell esds are taken into account in the estimation of
distances, angles and torsion angles
;

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
C1 C2 1.5318(19) . . no
C1 C9 1.4870(17) . . no
C1 C13 1.3551(17) . . no
C2 C3 1.559(2) . . no
C2 C10 1.538(2) . . no
C3 C4 1.511(2) . . no
C4 C5 1.4006(18) . . no
C4 C9 1.4111(17) . . no
C5 C6 1.396(2) . . no
C5 C11 1.512(2) . . no
C6 C7 1.393(2) . . no
C7 C8 1.409(2) . . no
C8 C9 1.4080(19) . . no
C8 C12 1.510(2) . . no
C13 C14 1.5362(18) . . no
C13 C21 1.4807(18) . . no
C14 C15 1.555(2) . . no
C14 C22 1.538(2) . . no
C15 C16 1.511(2) . . no
C16 C17 1.3986(19) . . no
C16 C21 1.4113(17) . . no
C17 C18 1.398(2) . . no
C17 C23 1.512(2) . . no
C18 C19 1.393(2) . . no
C19 C20 1.406(2) . . no
C20 C21 1.4084(18) . . no
C20 C24 1.509(2) . . no
C2 H2 0.983(15) . . no
C3 H3 1.001(16) . . no
C3 H3' 1.025(17) . . no
C6 H6 0.983(19) . . no
C7 H7 1.005(16) . . no
C10 H10 0.977(19) . . no
C10 H10' 1.017(18) . . no
C10 H10" 1.015(17) . . no
C11 H11 1.01(2) . . no
C11 H11' 1.02(2) . . no
C11 H11" 0.998(18) . . no
C12 H12 1.005(17) . . no
C12 H12' 1.016(18) . . no
C12 H12" 0.998(18) . . no
C14 H14 0.984(16) . . no
C15 H15 1.030(19) . . no
C15 H15' 1.030(17) . . no
C18 H18 0.990(18) . . no
C19 H19 0.999(18) . . no
C22 H22 0.993(16) . . no
```

```
C22 H22' 0.976(17) . . no
C22 H22" 1.030(18) . . no
C23 H23 0.994(18) . . no
C23 H23' 1.00(2) . . no
C23 H23" 0.97(2) . . no
C24 H24 0.988(17) . . no
C24 H24' 1.003(18) . . no
C24 H24" 0.987(19) . . no

loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
C2 C1 C9 105.25(10) . . . no
C2 C1 C13 123.19(12) . . . no
C9 C1 C13 131.44(12) . . . no
C1 C2 C3 101.88(11) . . . no
C1 C2 C10 112.30(11) . . . no
C3 C2 C10 111.21(13) . . . no
C2 C3 C4 102.80(12) . . . no
C3 C4 C5 127.49(12) . . . no
C3 C4 C9 110.18(11) . . . no
C5 C4 C9 122.32(12) . . . no
C4 C5 C6 116.42(12) . . . no
C4 C5 C11 121.41(13) . . . no
C6 C5 C11 122.17(13) . . . no
C5 C6 C7 121.77(14) . . . no
C6 C7 C8 122.31(14) . . . no
C7 C8 C9 116.24(12) . . . no
C7 C8 C12 119.43(13) . . . no
C9 C8 C12 124.20(12) . . . no
C1 C9 C4 108.32(11) . . . no
C1 C9 C8 130.62(11) . . . no
C4 C9 C8 120.67(11) . . . no
C1 C13 C14 123.50(11) . . . no
C1 C13 C21 131.57(12) . . . no
C14 C13 C21 104.72(10) . . . no
C13 C14 C15 101.31(11) . . . no
C13 C14 C22 112.42(11) . . . no
C15 C14 C22 110.68(11) . . . no
C14 C15 C16 102.51(12) . . . no
C15 C16 C17 128.02(12) . . . no
C15 C16 C21 109.79(12) . . . no
C17 C16 C21 122.15(12) . . . no
C16 C17 C18 116.30(12) . . . no
C16 C17 C23 121.86(13) . . . no
C18 C17 C23 121.83(13) . . . no
C17 C18 C19 121.91(14) . . . no
C18 C19 C20 122.31(14) . . . no
C19 C20 C21 116.02(12) . . . no
C19 C20 C24 120.07(12) . . . no
C21 C20 C24 123.75(11) . . . no
C13 C21 C16 108.41(11) . . . no
C13 C21 C20 130.13(11) . . . no
C16 C21 C20 121.03(11) . . . no
C1 C2 H2 112.7(9) . . . no
```

```
C3 C2 H2 110.3(10) . . . no
C10 C2 H2 108.3(9) . . . no
C2 C3 H3 111.9(10) . . . no
C2 C3 H3' 113.1(9) . . . no
C4 C3 H3 114.5(9) . . . no
C4 C3 H3' 109.1(9) . . . no
H3 C3 H3' 105.7(14) . . . no
C5 C6 H6 118.2(10) . . . no
C7 C6 H6 120.1(10) . . . no
C6 C7 H7 121.6(10) . . . no
C8 C7 H7 116.1(10) . . . no
C2 C10 H10 109.2(11) . . . no
C2 C10 H10' 111.0(10) . . . no
C2 C10 H10" 112.2(9) . . . no
H10 C10 H10' 111.0(14) . . . no
H10 C10 H10" 105.3(14) . . . no
H10' C10 H10" 107.9(13) . . . no
C5 C11 H11 111.4(10) . . . no
C5 C11 H11' 110.2(13) . . . no
C5 C11 H11" 112.2(11) . . . no
H11 C11 H11' 111.9(16) . . . no
H11 C11 H11" 104.8(15) . . . no
H11' C11 H11" 106.2(17) . . . no
C8 C12 H12 112.1(10) . . . no
C8 C12 H12' 109.7(11) . . . no
C8 C12 H12" 111.7(10) . . . no
H12 C12 H12' 106.3(14) . . . no
H12 C12 H12" 107.8(15) . . . no
H12' C12 H12" 109.0(15) . . . no
C13 C14 H14 111.9(9) . . . no
C15 C14 H14 112.0(10) . . . no
C22 C14 H14 108.5(10) . . . no
C14 C15 H15 111.4(10) . . . no
C14 C15 H15' 111.8(9) . . . no
C16 C15 H15 115.0(10) . . . no
C16 C15 H15' 110.3(9) . . . no
H15 C15 H15' 105.9(14) . . . no
C17 C18 H18 118.4(10) . . . no
C19 C18 H18 119.7(11) . . . no
C18 C19 H19 119.6(10) . . . no
C20 C19 H19 118.1(10) . . . no
C14 C22 H22 110.0(10) . . . no
C14 C22 H22' 110.0(10) . . . no
C14 C22 H22" 112.2(9) . . . no
H22 C22 H22' 110.2(13) . . . no
H22 C22 H22" 108.4(14) . . . no
H22' C22 H22" 106.1(14) . . . no
C17 C23 H23 112.1(11) . . . no
C17 C23 H23' 114.2(14) . . . no
C17 C23 H23" 113.1(14) . . . no
H23 C23 H23' 106.8(17) . . . no
H23 C23 H23" 106.2(18) . . . no
H23' C23 H23" 103.7(19) . . . no
C20 C24 H24 111.3(10) . . . no
C20 C24 H24' 110.0(10) . . . no
C20 C24 H24" 108.9(11) . . . no
H24 C24 H24' 108.9(14) . . . no
H24 C24 H24" 106.5(14) . . . no
H24' C24 H24" 111.3(14) . . . no

loop_
```

```
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
C9 C1 C2 C3 -32.87(13) . . . . no
C9 C1 C2 C10 86.20(13) . . . . no
C13 C1 C2 C3 143.36(13) . . . . no
C13 C1 C2 C10 -97.57(15) . . . . no
C2 C1 C9 C4 22.07(13) . . . . no
C2 C1 C9 C8 -150.56(13) . . . . no
C13 C1 C9 C4 -153.72(13) . . . . no
C13 C1 C9 C8 33.7(2) . . . . no
C2 C1 C13 C14 19.45(18) . . . . no
C2 C1 C13 C21 -166.62(12) . . . . no
C9 C1 C13 C14 -165.41(12) . . . . no
C9 C1 C13 C21 8.5(2) . . . . no
C1 C2 C3 C4 31.31(13) . . . . no
C10 C2 C3 C4 -88.53(13) . . . . no
C2 C3 C4 C5 159.01(13) . . . . no
C2 C3 C4 C9 -19.47(15) . . . . no
C3 C4 C5 C6 -175.62(14) . . . . no
C3 C4 C5 C11 4.3(2) . . . . no
C9 C4 C5 C6 2.69(19) . . . . no
C9 C4 C5 C11 -177.44(13) . . . . no
C3 C4 C9 C1 -1.25(14) . . . . no
C3 C4 C9 C8 172.25(12) . . . . no
C5 C4 C9 C1 -179.82(11) . . . . no
C5 C4 C9 C8 -6.32(19) . . . . no
C4 C5 C6 C7 1.3(2) . . . . no
C11 C5 C6 C7 -178.59(15) . . . . no
C5 C6 C7 C8 -1.7(2) . . . . no
C6 C7 C8 C9 -1.8(2) . . . . no
C6 C7 C8 C12 174.09(15) . . . . no
C7 C8 C9 C1 177.45(13) . . . . no
C7 C8 C9 C4 5.59(19) . . . . no
C12 C8 C9 C1 1.8(2) . . . . no
C12 C8 C9 C4 -170.02(13) . . . . no
C1 C13 C14 C15 140.27(13) . . . . no
C1 C13 C14 C22 -101.56(14) . . . . no
C21 C13 C14 C15 -35.04(12) . . . . no
C21 C13 C14 C22 83.13(13) . . . . no
C1 C13 C21 C16 -151.32(13) . . . . no
C1 C13 C21 C20 36.3(2) . . . . no
C14 C13 C21 C16 23.46(13) . . . . no
C14 C13 C21 C20 -148.91(12) . . . . no
C13 C14 C15 C16 33.43(12) . . . . no
C22 C14 C15 C16 -85.99(13) . . . . no
C14 C15 C16 C17 156.80(12) . . . . no
C14 C15 C16 C21 -20.90(14) . . . . no
C15 C16 C17 C18 -175.21(14) . . . . no
C15 C16 C17 C23 5.6(2) . . . . no
C21 C16 C17 C18 2.23(18) . . . . no
C21 C16 C17 C23 -177.01(12) . . . . no
C15 C16 C21 C13 -1.30(14) . . . . no
C15 C16 C21 C20 171.90(12) . . . . no
```

```
C17 C16 C21 C13 -179.15(11) . . . . no
C17 C16 C21 C20 -5.96(18) . . . . no
C16 C17 C18 C19 2.0(2) . . . . no
C23 C17 C18 C19 -178.81(14) . . . . no
C17 C18 C19 C20 -2.6(2) . . . . no
C18 C19 C20 C21 -1.0(2) . . . . no
C18 C19 C20 C24 174.53(14) . . . . no
C19 C20 C21 C13 176.67(13) . . . . no
C19 C20 C21 C16 5.12(18) . . . . no
C24 C20 C21 C13 1.3(2) . . . . no
C24 C20 C21 C16 -170.23(12) . . . . no

loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
_geom_contact_publ_flag
C1 C24 3.398(2) . . no
C5 C12 3.530(2) . 1_565 no
C8 C20 3.5817(19) . . no
C8 C21 3.5896(19) . . no
C8 C24 3.262(2) . . no
C9 C20 3.5995(19) . . no
C9 C24 3.213(2) . . no
C12 C13 3.410(2) . . no
C12 C24 3.491(3) . . no
C12 C5 3.530(2) . 1_545 no
C12 C21 3.191(2) . . no
C12 C20 3.237(2) . . no
C13 C12 3.410(2) . . no
C17 C24 3.487(2) . 1_545 no
C20 C12 3.237(2) . . no
C20 C9 3.5995(19) . . no
C20 C8 3.5817(19) . . no
C21 C12 3.191(2) . . no
C21 C8 3.5896(19) . . no
C24 C17 3.487(2) . 1_565 no
C24 C8 3.262(2) . . no
C24 C12 3.491(3) . . no
C24 C9 3.213(2) . . no
C24 C1 3.398(2) . . no
C1 H24' 2.906(17) . . no
C1 H12" 2.943(18) . . no
C2 H14 2.774(17) . . no
C3 H11" 3.067(19) . . no
C3 H11 3.072(19) . . no
C4 H10 2.924(18) . . no
C4 H12" 3.087(18) . 1_565 no
C5 H12' 3.073(17) . 1_565 no
C5 H11 3.039(19) . 6_545 no
C7 H7 2.986(16) . 7_556 no
C8 H11" 2.918(18) . 1_545 no
C8 H24" 2.596(19) . . no
C9 H10 2.880(18) . . no
C9 H24' 2.878(16) . . no
C9 H24" 2.892(18) . . no
C10 H14 3.042(16) . . no
C11 H3 2.941(16) . . no
C11 H11 3.099(18) . 6_555 no
```

C12 H24" 2.905(18) . . no
C13 H24' 2.884(18) . . no
C13 H12" 2.940(18) . . no
C14 H2 2.816(17) . . no
C15 H23' 3.04(2) . . no
C16 H24' 3.078(17) . 1_545 no
C16 H22 2.853(17) . . no
C17 H24' 3.087(16) . 1_545 no
C17 H24 3.076(17) . 1_545 no
C18 H23" 3.06(2) . 3_556 no
C20 H23 2.772(19) . 1_565 no
C20 H12 2.569(16) . . no
C21 H12 2.869(17) . . no
C21 H12" 2.847(19) . . no
C21 H23 3.079(19) . 1_565 no
C21 H22 2.845(16) . . no
C22 H18 3.089(18) . 4_554 no
C23 H15 2.966(18) . . no
C24 H12 2.923(17) . . no
C24 H23 3.027(19) . 1_565 no
H2 C14 2.816(17) . . no
H2 H14 2.48(2) . . no
H2 H22" 2.59(2) . . no
H3 C11 2.941(16) . . no
H3 H10' 2.50(2) . . no
H3 H11 2.59(3) . . no
H6 H11' 2.39(3) . . no
H6 H6 2.49(3) . 7_566 no
H7 H12' 2.36(3) . . no
H7 C7 2.986(16) . 7_556 no
H7 H7 2.43(2) . 7_556 no
H10 C4 2.924(18) . . no
H10 C9 2.880(18) . . no
H10' H3 2.50(2) . . no
H10' H24" 2.47(2) . 4_564 no
H10" H14 2.47(2) . . no
H11 C3 3.072(19) . . no
H11 H3 2.59(3) . . no
H11 C5 3.039(19) . 6_555 no
H11 C11 3.099(18) . 6_545 no
H11' H6 2.39(3) . . no
H11" C3 3.067(19) . . no
H11" C8 2.918(18) . 1_565 no
H12 C20 2.569(16) . . no
H12 C21 2.869(17) . . no
H12 C24 2.923(17) . . no
H12 H24" 2.38(3) . . no
H12' C5 3.073(17) . 1_545 no
H12' H7 2.36(3) . . no
H12" C1 2.943(18) . . no
H12" C4 3.087(18) . 1_545 no
H12" C13 2.940(18) . . no
H12" C21 2.847(19) . . no
H14 C2 2.774(17) . . no
H14 C10 3.042(16) . . no
H14 H2 2.48(2) . . no
H14 H10" 2.47(2) . . no
H15 C23 2.966(18) . . no
H15 H22' 2.49(3) . . no
H15 H23' 2.55(3) . . no
H15 H23' 2.31(3) . 2_555 no

```
H15' H22" 2.54(2) . 1_545 no
H18 H23" 2.44(3) . . no
H18 C22 3.089(18) . 4_555 no
H18 H22' 2.29(3) . 4_555 no
H19 H24 2.43(2) . . no
H19 H22" 2.38(2) . 4_565 no
H22 C16 2.853(17) . . no
H22 C21 2.845(16) . . no
H22 H23 2.52(2) . 1_565 no
H22' H15 2.49(3) . . no
H22' H18 2.29(3) . 4_554 no
H22" H2 2.59(2) . . no
H22" H15' 2.54(2) . 1_565 no
H22" H19 2.38(2) . 4_564 no
H23 C20 2.772(19) . 1_545 no
H23 C21 3.079(19) . 1_545 no
H23 C24 3.027(19) . 1_545 no
H23 H22 2.52(2) . 1_545 no
H23' C15 3.04(2) . . no
H23' H15 2.55(3) . . no
H23' H15 2.31(3) . 2_555 no
H23" H18 2.44(3) . . no
H23" C18 3.06(2) . 3_556 no
H24 C17 3.076(17) . 1_565 no
H24 H19 2.43(2) . . no
H24' C1 2.906(17) . . no
H24' C9 2.878(16) . . no
H24' C13 2.884(18) . . no
H24' C16 3.078(17) . 1_565 no
H24' C17 3.087(16) . 1_565 no
H24" C8 2.596(19) . . no
H24" C9 2.892(18) . . no
H24" C12 2.905(18) . . no
H24" H12 2.38(3) . . no
H24" H10' 2.47(2) . 4_565 no

# Loop Mechanism for Extra Tables(s)

#loop_
#_publ_manuscript_incl_extra_item
#'_geom_extra_tableA_col_1'
#'_geom_extra_tableA_col_2'
#'_geom_extra_tableA_col_3'
#'_geom_extra_table_head_A'
#'_geom_table_footnote_A'
#'_geom_extra_tableB_col_1'
#'_geom_extra_tableB_col_2'
#'_geom_extra_tableB_col_3'
#'_geom_extra_table_head_B'
#'_geom_table_footnote_B'

#
#loop_
#_geom_extra_tableA_col_1
#_geom_extra_tableA_col_2
#_geom_extra_tableA_col_3
# ? ? ?

#
#loop_
#_geom_extra_tableB_col_1
```

```
#_geom_extra_tableB_col_2
#_geom_extra_tableB_col_3
# ? ? ?

#
#_geom_table_footnote_A
#;
# ?
#;

#
#_geom_table_footnote_B
#;
# ?
#;

#
#_geom_table_footnote_A
#;
# ?
#;

#
#_geom_table_footnote_B
#;
# ?
#;

#===END of Crystallographic Information File
```